



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4BIB / pdb_00004bib
Title : Crystal Structures of Ask1-inhibitor Complexes
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Deposited on : 2013-04-10
Resolution : 2.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

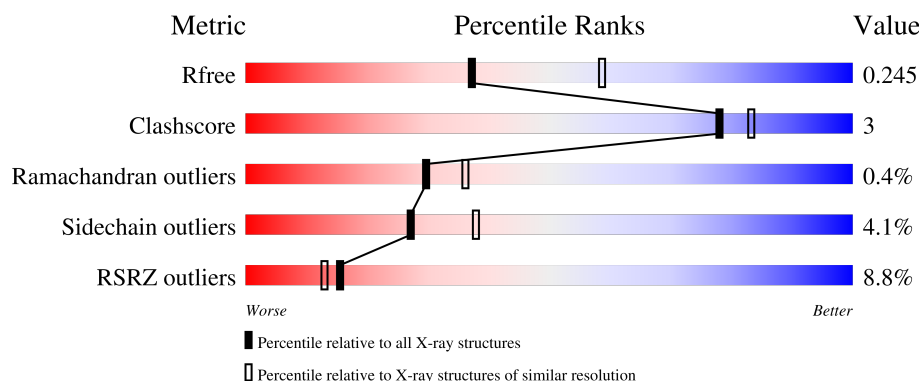
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	
1	B	318	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4206 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

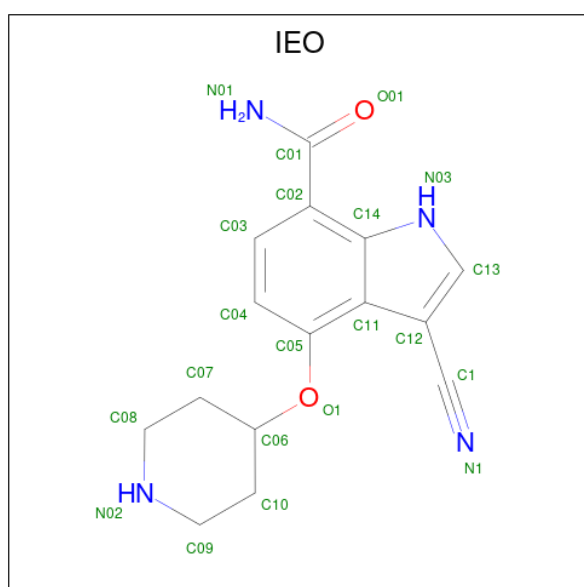
- Molecule 1 is a protein called MITOGEN-ACTIVATED PROTEIN KINASE KINASE KINASE 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	1	0
			1987	1281	324	373	9			
1	B	258	Total	C	N	O	S	0	1	0
			1990	1280	324	377	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	838	GLU	THR	engineered mutation	UNP Q99683
B	838	GLU	THR	engineered mutation	UNP Q99683

- Molecule 2 is 3-cyano-4-(piperidin-4-yloxy)-1H-indole-7-carboxamide (CCD ID: IEO) (formula: C₁₅H₁₆N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	15	4	2		
2	B	1	Total	C	N	O	0	0
			21	15	4	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	59	Total	O	0	0
			59	59		

- Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE KINASE KINASE 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.95Å 77.95Å 418.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.71 – 2.43 30.71 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.71-2.43) 99.7 (30.71-2.43)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.201 , 0.239 0.203 , 0.245	Depositor DCC
R_{free} test set	1511 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4206	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IEO, GOL, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.90	0/2030	1.34	10/2739 (0.4%)
1	B	0.80	0/2036	1.33	10/2752 (0.4%)
All	All	0.85	0/4066	1.33	20/5491 (0.4%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	LEU	N-CA-C	7.33	121.30	110.30
1	A	678	ASP	CA-C-N	6.77	129.66	120.38
1	A	678	ASP	C-N-CA	6.77	129.66	120.38
1	A	809	VAL	CB-CA-C	6.19	118.10	110.73
1	B	882	TYR	CA-C-N	5.72	127.95	120.28
1	B	882	TYR	C-N-CA	5.72	127.95	120.28
1	A	744	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	842	THR	CA-C-N	5.43	127.50	120.44
1	A	842	THR	C-N-CA	5.43	127.50	120.44
1	A	671	LEU	N-CA-C	5.42	117.14	108.41
1	B	852	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	904	PRO	CA-C-N	5.33	127.68	120.38
1	A	904	PRO	C-N-CA	5.33	127.68	120.38
1	B	670	LEU	CA-C-N	5.32	129.71	121.26
1	B	670	LEU	C-N-CA	5.32	129.71	121.26
1	B	729	HIS	CA-C-N	5.24	127.56	120.38
1	B	729	HIS	C-N-CA	5.24	127.56	120.38
1	B	678	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	922	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	678	ASP	CA-CB-CG	5.11	117.71	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	1938	11	0
1	B	1990	0	1929	8	0
2	A	21	0	16	1	0
2	B	21	0	16	2	0
3	A	12	0	16	2	0
4	A	8	0	6	0	0
4	B	4	0	3	0	0
5	A	104	0	0	1	0
5	B	59	0	0	0	0
All	All	4206	0	3924	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:GLU:HG2	1:A:923:PRO:HG3	1.68	0.75
2:B:1941:IEO:H071	2:B:1941:IEO:H04	1.72	0.70
1:A:900:HIS:NE2	3:A:1941:GOL:H32	2.18	0.59
1:B:869:CYS:HB3	1:B:880:PRO:HG3	1.85	0.58
2:B:1941:IEO:H071	2:B:1941:IEO:C04	2.34	0.57
1:B:729:HIS:HE1	1:B:738:VAL:O	1.90	0.55
1:A:725:GLU:CG	1:A:824:GLY:HA2	2.37	0.55
1:A:710:GLU:HG2	1:A:751:LYS:HG2	1.89	0.54
1:A:844:GLN:HG2	5:A:2073:HOH:O	2.08	0.53
1:B:840:THR:HG23	1:B:846:MET:HE1	1.93	0.50
1:B:849:GLU:HG2	1:B:850:ILE:HD12	1.95	0.49
1:B:679:GLU:H	1:B:679:GLU:HG3	1.43	0.48
1:A:807:ASP:O	2:A:1940:IEO:H082	2.13	0.48
3:A:1941:GOL:H31	3:A:1943:GOL:O3	2.14	0.47
1:B:849:GLU:O	1:B:853:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:GLU:HG2	1:A:824:GLY:HA2	1.96	0.46
1:B:706:ILE:HD12	1:B:753:PHE:HD2	1.82	0.45
1:A:802:ARG:HH12	1:A:837:GLU:HA	1.81	0.45
1:A:730:LYS:HA	1:A:740:TYR:CD1	2.55	0.42
1:A:869:CYS:HB3	1:A:880:PRO:HG3	2.02	0.41
1:B:688:LYS:HG2	1:B:693:ILE:HG12	2.01	0.41
1:A:922:ASP:HA	1:A:923:PRO:HD2	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/318 (78%)	239 (96%)	8 (3%)	2 (1%)	16	18
1	B	253/318 (80%)	243 (96%)	10 (4%)	0	100	100
All	All	502/636 (79%)	482 (96%)	18 (4%)	2 (0%)	30	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	747	ASN
1	A	822	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/274 (75%)	199 (97%)	7 (3%)	32	45
1	B	206/274 (75%)	196 (95%)	10 (5%)	22	31
All	All	412/548 (75%)	395 (96%)	17 (4%)	27	38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	671	LEU
1	A	698	ARG
1	A	725	GLU
1	A	737	ILE
1	A	809	VAL
1	A	849	GLU
1	A	939	LYS
1	B	671	LEU
1	B	679	GLU
1	B	710	GLU
1	B	733	LYS
1	B	737	ILE
1	B	768	SER
1	B	809	VAL
1	B	825	THR
1	B	910	GLU
1	B	916	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	680	ASN
1	A	756	GLN
1	A	798	GLN
1	B	729	HIS
1	B	756	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACT	B	1942	-	3,3,3	1.55	0	3,3,3	0.72	0
4	ACT	A	1942	-	3,3,3	1.15	0	3,3,3	0.59	0
2	IEO	A	1940	-	22,23,23	0.83	1 (4%)	27,32,32	1.13	2 (7%)
4	ACT	A	1944	-	3,3,3	1.19	0	3,3,3	0.96	0
3	GOL	A	1941	-	5,5,5	0.93	0	5,5,5	0.94	0
2	IEO	B	1941	-	22,23,23	0.78	1 (4%)	27,32,32	1.07	1 (3%)
3	GOL	A	1943	-	5,5,5	0.44	0	5,5,5	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1941	-	-	4/4/4/4	-
2	IEO	B	1941	-	-	0/8/18/18	1/3/3/3
3	GOL	A	1943	-	-	0/4/4/4	-
2	IEO	A	1940	-	-	0/8/18/18	1/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1941	IEO	C13-C12	-3.06	1.34	1.38
2	A	1940	IEO	C13-C12	-2.71	1.35	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1941	IEO	C14-C11-C12	-3.50	105.13	106.80
2	A	1940	IEO	C14-C11-C12	-3.10	105.32	106.80
2	A	1940	IEO	O1-C06-C10	-2.22	103.14	108.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1941	GOL	O1-C1-C2-C3
3	A	1941	GOL	C1-C2-C3-O3
3	A	1941	GOL	O2-C2-C3-O3
3	A	1941	GOL	O1-C1-C2-O2

All (2) ring outliers are listed below:

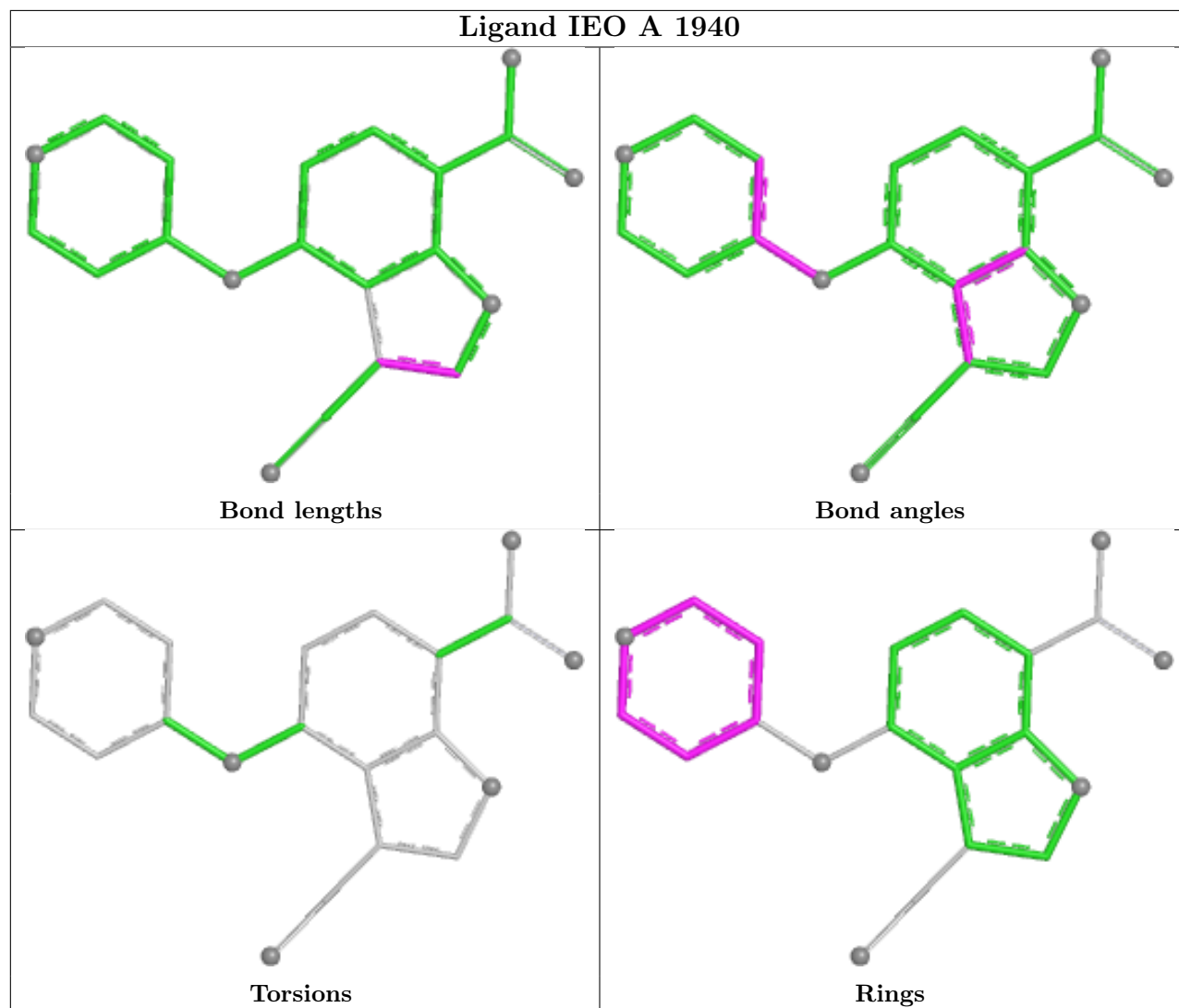
Mol	Chain	Res	Type	Atoms
2	B	1941	IEO	C06-C07-C08-C09-C10-N02
2	A	1940	IEO	C06-C07-C08-C09-C10-N02

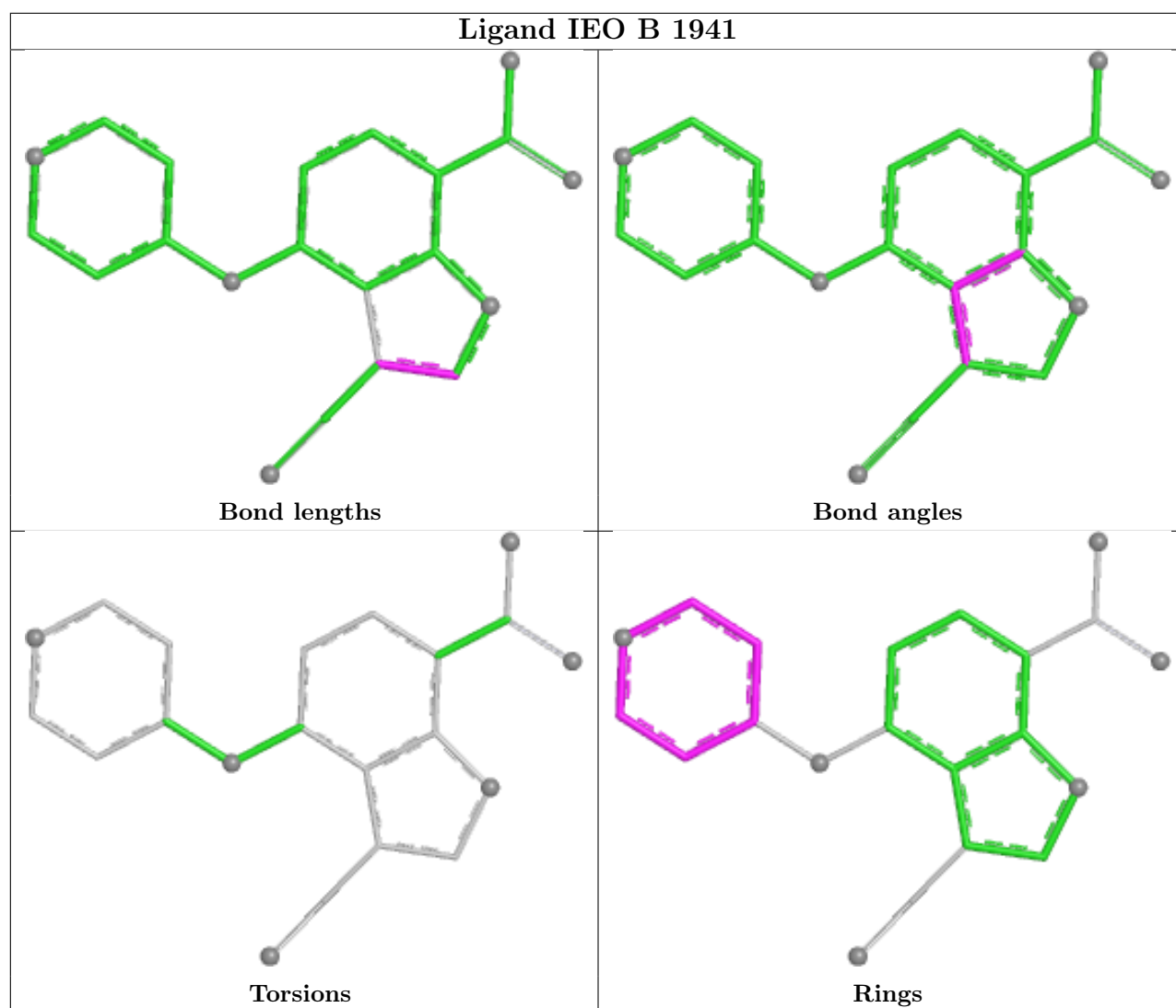
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1940	IEO	1	0
3	A	1941	GOL	2	0
2	B	1941	IEO	2	0
3	A	1943	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	254/318 (79%)	0.14	24 (9%) 14 11	23, 41, 84, 113	1 (0%)
1	B	258/318 (81%)	0.49	21 (8%) 18 15	33, 55, 92, 115	1 (0%)
All	All	512/636 (80%)	0.32	45 (8%) 15 13	23, 48, 90, 115	2 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	940	VAL	7.3
1	A	670	LEU	5.9
1	B	670	LEU	5.4
1	B	714	ARG	5.2
1	A	828	ARG	4.8
1	A	939	LYS	4.5
1	B	723	HIS	4.4
1	B	840	THR	4.4
1	B	691	TYR	4.1
1	A	827	LYS	4.1
1	A	724	GLU	3.9
1	A	691	TYR	3.7
1	A	722	LEU	3.6
1	B	858	TYR	3.4
1	A	690	THR	3.4
1	B	829	LEU	3.3
1	A	713	GLU	3.1
1	B	720	GLN	3.0
1	B	825	THR	3.0
1	B	722	LEU	3.0
1	A	824	GLY	3.0
1	A	837	GLU	2.9
1	A	726	ILE	2.8
1	B	839	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	823	PHE	2.8
1	A	711	ILE	2.7
1	A	723	HIS	2.6
1	B	861	ALA	2.6
1	B	851	ILE	2.5
1	B	719	SER	2.5
1	A	727	ALA	2.5
1	B	855	PRO	2.3
1	A	768	SER	2.3
1	B	690	THR	2.2
1	B	748	GLY	2.2
1	B	824	GLY	2.2
1	A	750	ILE	2.2
1	A	825	THR	2.2
1	B	853	LYS	2.2
1	A	826	SER	2.2
1	A	728	LEU	2.1
1	A	730	LYS	2.1
1	A	852	ASP	2.1
1	B	936	GLU	2.0
1	A	731	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	1944	4/4	0.83	0.16	46,48,49,49	0
4	ACT	A	1942	4/4	0.85	0.17	59,62,62,63	0

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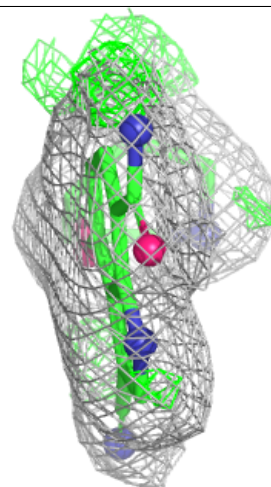
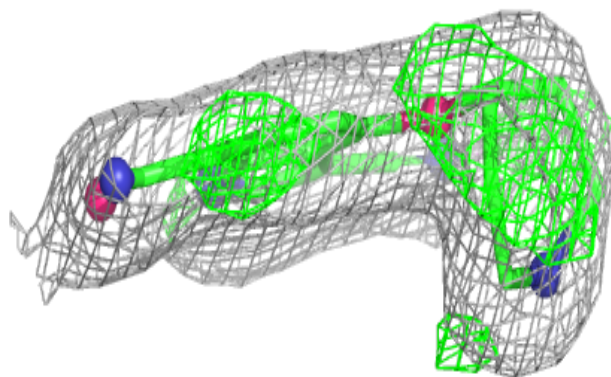
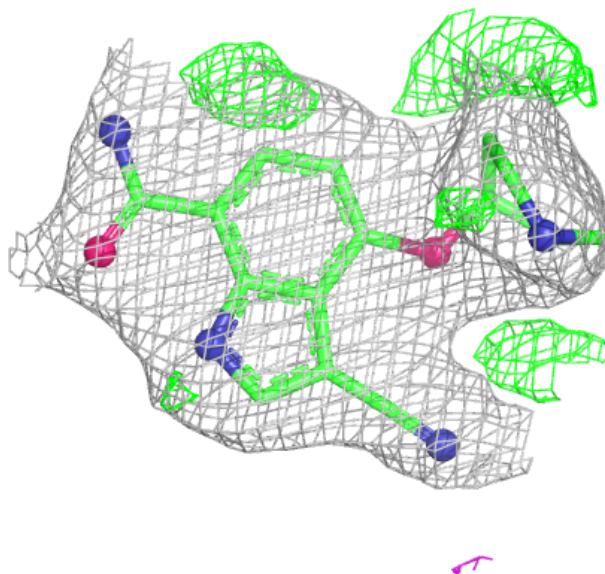
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1941	6/6	0.85	0.13	56,57,57,57	0
3	GOL	A	1943	6/6	0.86	0.20	81,81,82,83	0
4	ACT	B	1942	4/4	0.86	0.15	46,48,49,50	0
2	IEO	B	1941	21/21	0.87	0.12	41,45,54,55	0
2	IEO	A	1940	21/21	0.89	0.11	33,37,42,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

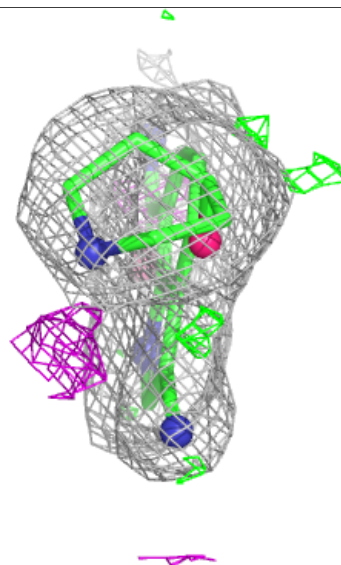
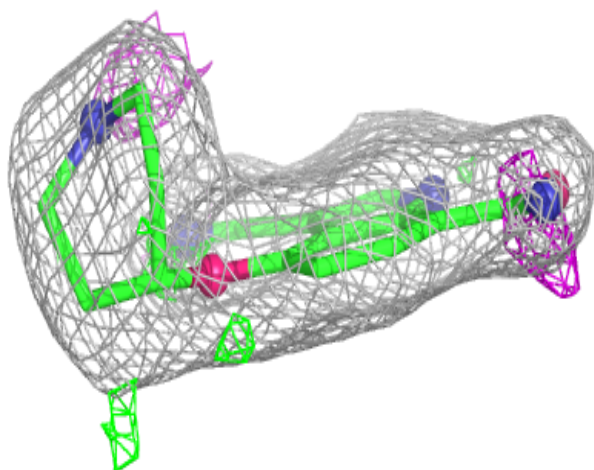
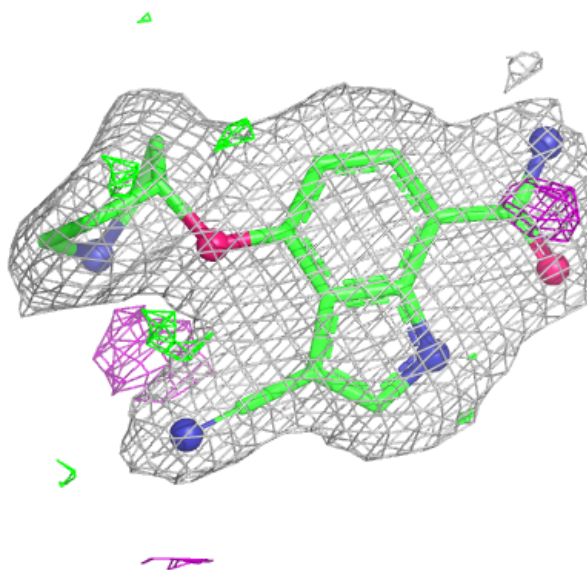
Electron density around IEO B 1941:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IEO A 1940:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.